Strain-induced modulation of band structure of Silicon

S. Zh. Karazhanov*,[1,2] A. Davletova,[2] and A. Ulyashin[1]

[1]*Institute for Energy Technology, P.O.Box 40, NO-2027 Kjeller, Norway*

[2]*Physical-Technical Institute, 2B Mavlyanov St., 700084 Tashkent, Uzbekistan*

This work presents ab initio study of strain-induced modulation of band structure of Si. It is shown that at straining pressures >12 GPa band structure of Si can be turned from indirect to direct. Both the bottommost conduction band and topmost valence band are located at the Γ point. The conduction band minimum at the Γ point of the strained Si is found to be much more dispersive than that at the X point of the unstressed Si. Consequently, electrical conductivity through the Γ valley is suggested to be more superior than the X point of the unstressed Si. Barrier height, which is needed to transfer electrons in the Γ point to X/L points or from X/L to Γ point have been calculated. The results have been applied to explain peculiarities of electronic structure and light emission of Si based materials containing dislocations and voids.

PACS: 85.30.De, 85.60.Bt, 85.60.Jb

Keywords: strained Si, voids, dislocation engineering, electronic structure

***Corresponding author:** e-mail:smagul.karazhanov@ife.no

1. Introduction

Due to many technologically important properties and availability, the Si based structures still remain to be the basic materials of modern semiconductor electronics. Properties of the Si based devices can be modulated by impurities, defects, interfaces, spin, pressure, strain etc. The latter can qualitatively change photoelectrical and electrophysical properties of Si. Such strains can be available in close vicinity of, for example, dislocations or nanophases. Magnitude and sign of the dislocation-induced strain has been estimated for Si within the elastic theory of dislocations and is found to be in the range 25-50 GPa.[1] The strain was suggested to cause an increase of the Si band gap of 325-750 meV. It should be noted that the stress 25-50 GPa is quite large. In case of Si such a stress can cause not only increase of the Si-Si bond length and the fundamental band gap, but also it can be sufficient to modulate the band structure qualitatively, e.g. to turn it from indirect to direct.[2] Furthermore, it forms a potential barrier and causes carrier confinement.[1] However, magnitude of the band offset between the strained and bulk Si has not yet been estimated. Although the dislocation-related luminescence in Si consisting of D1, D2, D3, and D4 lines is important for applications in light emitting diodes, the origin of the D1 and D2 luminescence lines still is unknown.[3] Clarification of these points would be useful to find the ways of increasing the efficiency of the dislocation-related luminescence, the luminescence temperature, in understanding, purposeful controlling and exploiting dislocations as well as extending the list of their applications.

Here it should be noted that the strain field around dislocations can be the source for gettering the impurities, which affect electrical conductivity of Si. These problems initiated *ab initio* studies of interaction of H with dislocations,[4, 5] passivation of the

defects by H,[6] effect of extended defects on properties of intrinsic and extrinsic point defects.[7] H impurity can be useful not only to passivate deep traps and enhance electrical conductivity, but also to reduce strain around external defects.

Although the elongated Si-Si bonds can be formed in whole regions in ion-implanted single-crystalline, poly- and multi-crystalline Si, porous Si, a-Si:H, voids, dislocations or nanophases, there was no attempt to correlate the origin of the luminescence feature of the above phases of Si with existence of the regions with elongated Si-Si bonds. Such an attempt can be useful to solve the problems such as difference in energy value of the photoluminescence (PL) peak (see, e.g., Ref.[8]) and intensity and as well as order of locations of the peaks experimentally observed by different authors in dislocation containing Si. If commonly four D1-D4 peaks are observed[9] in PL spectra in the order of the increasing energy, only D1 and D2 have been observed in O and Si implanted single crystalline Si,[10, 11] D2-D4 peaks in gamma-irradiated and hydrogen plasma treated multicrystalline Si,[12] more than four peaks in hydrogen and helium implanted Si,[13] D1 line in hydrogen and helium implanted Czochralski Si[8] and a-Si:H,[14] etc.

It is worth to mention here some other findings, which can be supportive to our results in this work. One of them is the suggestion to relate the origin of the Staebler-Wronski effect with voids and elongated Si-Si bonds.[15, 16] The other one is the first-principles studies for hydrogen-passivated single-crystalline Si nanotubes,[17] which report that band gap of the nanophases can be direct and some Si-Si bonds are elongated than those in the bulk Si. The PL in the spectral range around D1 peak has been observed experimentally in Si nanowires. Moreover, the luminescence efficiency of *a*-Si:H in this range is more advanced than that in *c*-Si due to structural disorder.[14, 18]

Pressure-induced variation of gap of Si has also been studied before both experimentally and theoretically by density functional theory (DFT) within local density approximation (LDA) and quasiparticle corrections.[19] It is found that although the computations within LDA underestimates the band gap by ~50-100% of the experimentally measured one, the pressure coefficients of the band gaps are accurate for carbon[20] and other group-IV elementary and III-V compound semiconductors.[21] Observation of photoluminescence in porous Si[22] has initiated *ab initio* studies[2] of the effect of lattice expansion on band edge levels of group-IV materials and it was found from that upon straining the Si with negative pressure ~15.5 GPa its band gap can be converted from indirect to direct. Similar result was obtained for Si by linear combination of Gaussian orbitals method (Ref.[23]) and by GW ("G" stands for one-particle Green's function as derived from many-body perturbation theory and "W" for Coulomb screened interactions) approximation.[24] However, in these studies effective masses related to the newly formed minimum at the Γ point, barrier heights to transfer conduction band electrons from/to X, Γ, and L points as well as band offset between strained and unstrained regions of Si have not been studied and relation of these results to luminescence, transport, and recombination properties of Si was not discussed.

The aim of the paper is to study electronic structure of Si for different strain values in the range 0-20 GPa as well as band structure of Si with a nanodot/nanowire from a void. We found that at strains >12 GPa band structure of Si can indeed be turned from indirect to direct with the bottommost conduction band (CB) and topmost valence band (VB) located at the Γ-point, (ii) conduction band electron effective mass related to the Γ-point is much smaller than that at the *X* and *L* points, (iii) band offset between the

strained and bulk has been calculated. Also, we discuss role of the results in electrical and optical properties of Si containing strained regions.

2. Computational details

VASP-PAW package[25, 26] has been used in the present study along with generalized-gradient approximation of Perdew-Wang[27]. Lattice relaxation was performed by using the conjugate gradient method. The plane-wave cutoff energy of 500 eV was used for all the calculations. The convergence was achieved when the forces acting on the atoms were smaller than 20 meV $Å^{-1}$ and the total energy difference between two consecutive iterations were < 10^{-6} eV. The convergence criteria and more details about the optical calculations were discussed in Ref. [28].

Self-consistent calculations were performed using a 10×10×10 mesh frame according to Monkhorst-Pack scheme for primitive unit cell of Si. The unit-cell vectors used are **a**=(0,1/2,1/2)*a*, **b**=(1/2,0,1/2)*a*, and **c**=(1/2,1/2,0)*a*, *a* is the cubic lattice constant, and there are four formula units per unit cell specified at (0,0,0) and (1/4,1/4,1/4). To study Si with a void in the form of a smallest quantum dot 2×2×2 supercell has been considered. Several atoms from the center of the supercell have been removed. To mimic Si with a quantum wire of a void 3×3×1 supercell has been prepared and a few lines from the center have been removed. The dangling bonds have not been passivated by H. The structures have been optimized.

Band offset (E_b) between strained and bulk Si has been calculated following the standard scheme[29] by the formula

$$E_b = \left(E_{bulk}^{VB} - E_{bulk}^{core}\right) - \left(E_{str}^{VB} - E_{str}^{core}\right). \quad (1)$$

Here E_{bulk}^{VB} and E_{str}^{VB} are the topmost VB for bulk and strained Si whereas E_{bulk}^{core} and E_{str}^{core} are the average electrostatic potentialsused as the reference level. To estimate the CB offset, band gap values calculated[24] within GW approximation have been used.

Effective masses have been calculated by:

$$\frac{1}{m_c(\mathrm{k})} = \frac{1}{h^2}\frac{\partial^2 E(\mathrm{k})}{\partial \mathrm{k}^2}\bigg|_{\mathrm{k}=\mathrm{k}_0} \qquad (2)$$

in the close vicinity of the band extremum in the energy range 25-300 meV[28]. As it was demonstrated for a number of III-V and II-VI semiconductors, the LDA calculations underestimate not only the band gap, but also the CB effective masses.[30, 31]

3. Results

3.1 Structural studies

Using the lattice parameter *a*=5.392 Å and positional parameters of Ref.[32] as input crystal lattice of Si has been optimized. The equilibrium lattice constant has been estimated from the minimum in dependence of the total energy on volume and found to be equal to *a*=5.27 Å, which was used as equilibrium lattice parameter. The dependence of the total energy on volume has been used to fit the universal equation of state and bulk modulus (B_0) and its first derivative (B_0') on pressure have been calculated, which is equal to B_0=89.50 GPa and B_0'=4.34, respectively. The calculated data are in good agreement with experimentally determined values B_0=97.82 GPa[33] and B_0'=4.09[34] as well as with theoretical results of Ref.[2, 24], which demonstrates that the computations are reliable.

3.2 Band structure and band gaps

To mimic strain-induced variation of band structure of Si we have performed electronic structure studies for different values of the lattice parameter. Figure 1 presents band structure for unstrained bulk Si with *P*=0 GPa and strained Si with straining pressure value of *P*=11.9 GPa. It is seen that distinct from the bulk Si with indirect band gap, the strained Si posses direct band gap with the bottommost CB and topmost VB located at the Γ point. The strain value *P*=11.9 GPa is in the range is smaller than 15.5 GPa of Ref. [2] and much smaller than lowest limit 20 GPa[1] estimated within the elasticity theory of dislocations. It indicates that the strain causes not only simply reduction/increase of the fundamental band gap, but can change it qualitatively by turning it from indirect to direct. Upon straining VB maximum at the Γ point remained unchanged. However, the CB extreme at the *L*, Γ, and *X* points have been changed drastically.

Figure 2 displays strain dependence of the band gaps E_g^L, E_g^Γ, and E_g^X related to the *L*, Γ, and *X* points, respectively. The band gaps have been calculated compared to the topmost VB as the reference point. It is seen that E_g^X increases, whereas E_g^L and E_g^Γ decrease with increasing the straining pressure. Decrease of E_g^Γ is faster than that of E_g^L. As a result at strains ≥12 GPa E_g^Γ can become smaller than E_g^L and Si becomes direct band gap material. Direct optical transitions in strained Si can be more enhanced than the unstrained Si.

It should also be noted that although band structure of Si has been turned from indirect to direct at moderate strains around 12 GPa, the band values E_g^X, E_g^L, and E_g^Γ are close to each other. It shows that both indirect and direct optical transitions can play

important role in optical properties of the strained Si around the fundamental absorption edge.

According to Figs. 1 and 2 the calculated band gaps have been underestimated. This shortcoming of the method comes out because of the well known deficiency of DFT. Nowadays there exist several ways to overcome it. One of them is rigid shift of all CB until the fundamental band gap established experimentally. To check whether this approach can be applied in this particular case we have studied pressure-induced variation of the fundamental band gap (Fig. 3) and compared with experimental results.[35] It is seen that the theoretically calculated and experimentally determined dependencies of the fundamental band gap on applied pressure are almost parallel. The calculated pressure coefficient of the fundamental band gap -18.0 meV/GPa is in reasonable agreement with experimentally established -14±1 meV/GPa[35] and -14±0.6 meV/GPa.[36], which indicates that the rigid shift technique can be applied for this particular pressure range.

As it is well known bottommost CB in unstrained bulk Si does not posses a well defined extremum. Distinguishing feature of strained Si is that such an extremum is at the Γ point. Dispersion around the newly formed well in the Γ point is much more dispersive than those at *L* and *X* points of the unstrained Si. Because of this feature electrical current transport by CB electrons through the Γ point is expected to be better than that through *X* and *L* points.

3.3 Effective masses

For comparative analysis of the band dispersion around the Γ point we have calculated carrier effective masses. The results are presented in Table I. Analysis of Table I shows

that the calculated CB and VB electron effective masses for unstrained bulk Si are in good agreement with experimental data. These findings indicate that the computations are reliable. Then the masses have been calculated for strained Si with turned band gap. It is seen in Table I that upon straining the VB masses have not been changed much. However, the CB electron mass at the Γ point is much smaller than that in the *X* point. Consequently, electrical parameters of well strained Si can be different than unstrained one.

3.4 Barrier heights

Analysis of the CB shows that the bottommost CB located at the *L* and *X* points are separated from that at the Γ point by a potential barrier $\Delta E^{L-\Gamma}$ and $\Delta E^{X-\Gamma}$, respectively. Similarly, the electrons located at the Γ valley can be transferred to L or X valley by overcoming the potential barrier $\Delta E^{\Gamma-L}$ and $\Delta E^{\Gamma-X}$, respectively. The barrier heights can be changed upon variation of the strain. In Figure 4 strain-induced variation of $\Delta E^{L-\Gamma}$, $\Delta E^{X-\Gamma}$, $\Delta E^{\Gamma-L}$, and $\Delta E^{\Gamma-X}$ have been presented. It is seen that $\Delta E^{L-\Gamma}$ and $\Delta E^{X-\Gamma}$ in pressurized Si is smaller than those of un-pressurized bulk Si. It shows that free carriers located at the *L* and *X* points of the strained Si can more easily e thermally activated and transferred to the valley in the Γ point than those of unstrained Si. Consequently, luminescence intensity coming from direct band to band transitions can increase with increasing the temperature.

The barrier heights $\Delta E^{\Gamma-L}$ and $\Delta E^{\Gamma-X}$ increase with increasing the strain. In the strain range from 11.4 to 12.2 GPa magnitude of the barriers can become be almost the same as their counterparts $\Delta E^{L-\Gamma}$ and $\Delta E^{X-\Gamma}$, respectively.

3.5 Band offset, bond length and volume

Upon straining topmost VB of Si can be shifted compared to unstrained Si. As a result between strained and unstrained Si band offset can be formed, which can effect on transport of electrical current. The band offset has been calculated between the strained and unstrained Si as a function of straining pressures. For the computation we followed the way discussed in Ref.[29]. Distinct from Ref.[29] we did not construct a supercell, because both strained and bulk material are from one and the same material. To make sure that our approach agrees with the standard one, we calculated the band offset for 24 atomic-layer wurtzite ZnSe/ZnTe superlattice. We found a valence band offset of 1.01 eV for the interface ZnSe/ZnTe, which is in very good agreement with the experimentally established 0.97±0.1 eV.[37] This gives us confidence that the way of estimation of the band offset is reliable.

Figure 5 demonstrates VB offset between strained and unstrained Si. It is seen that topmost VB of the strained Si is lower than that of the unstrained one. However, the band offset is small, so holes shall be accumulated in the unstrained part of Si. CB offset has been estimated using the band gap values of strained Si calculated[24] within GW approximation. It shows that CB electrons can be confined in the strained part of Si. If, as we noted upon analysis of band dispersion, electronic conductivity along the newly formed CB minimum of Si is more enhanced than that in bulk Si, carrier confinement around dislocations can explain the reason of the experimentally established result as to more enhanced electrical conductivity in Si along dislocations than that of bulk Si.[38, 39]

If the CB electrons accumulated in the strained region, then that region can attract the injected holes, which can enhance carrier recombination. If the recombination is radiative, then luminescence intensity can also be enhanced. Analysis of Fig. 5 shows

that depending on the straining pressure in the range from 0-12.5 GPa, band offset between CB of strained and unstrained Si can be different and be varied in the range 0-0.50 eV. That can explain why location of D1-D4 peaks of different Si samples differs each from other. Intensity of the luminescence can be controlled by deep level defects decorating the strained region. Furthermore, the CB electrons located in the strained part of Si can be can be thermally activated and be transferred to unstrained part of Si. Probability of this process increases with increasing temperature thus leading to reducing the luminescence intensity. That can explain the reason of thermal quenching of luminescence of Si. The CB offset range 0.0-0.50 eV (Fig. 5) is close to the experimentally determined activation energy range 0.16-0.35 eV for thermal quenching the D1 line .[3]

Figure 6 shows variation of the Si-Si bond length and volume of primitive unit cell of Si as a function of strain. It is seen that at strains >12 GPa Si-Si bond length is elongated so that it can be sufficient to cause turning of the band gap from indirect to direct.

4. Band structure of Si with a nanodot and nanowire formed by a void

The above discussed findings of this work indicate that the presence of strained region(s) in Si with elongated Si-Si bonds can drastically modulate band structure of Si. As mentioned in Introduction, such regions can be formed around dislocations, nanostructures, and voids. Here we shall demonstrate it in the example of Si with a vacancy and a void in the form of a nanodot and nanowire. The latter structures have been schematically presented in Fig. 7. Figure 8 displays number of Si-Si bonds as a function of the Si-Si bond length in the optimized structure of Si. It is seen that bond

length of some Si-Si bonds in the Si with a void in the form of a dot/wire exceeds that of strained Si with turned band structure. Band structures for the Si with the void-dot and void-wire are presented in Fig. 9. It is seen that band structures have been modified. For Si with a void wire it is of direct band gap. This result indicates that band structure of Si can be modulated depending on size and form of the void. The voids can be regarded as multi-vacancy complex and the results presented indicate to possibility of band-gap engineering by structural defects. Such voids can be formed in ion-implanted Si.[8, 13] The direct band gap of the group of atoms can be responsible for the luminescent features of the ion implanted Si, which previously have been ascribed to dislocations.

5. Discussion

As mentioned in Introduction, the strain region can be formed around dislocations. Consequently, the results presented can be related to dislocation engineered Si. For example, the result as to turning band structure of Si from indirect to direct can explain the reason for the enhancement of the radiative recombination in dislocation engineered Si than the unstrained one.[1] The finding that magnitude of the band gaps related of the *L*, Γ, and *X* points are close to each other indicates that both direct and indirect optical transitions can be almost the same. This can explain the experimental evidences as to observation of the phonon assisted transitions.[35] The result as to reduction of the barrier height to transfer CB electrons from *L*/*X* points into Γ with increasing the strain is also important. It indicates that upon increasing the temperature number of free carriers transferring from *L*/*X* points into Γ increases thus increasing the intensity of radiative direct optical transition. Consequently, this result can explain the experimentally

observed fact as to increase of the illumination intensity with increasing the temperature.

The idea of strained Si with direct band gap is consistent with the model[15, 16] relating the origin of the Staebler-Wronski effect in *a*-Si:H to an enormous number of voids in the sense that carrier recombination in direct band gap material is known to be much faster than those with indirect band gap. Furthermore, it explains why light-emitting feature of *a*-Si:H in the infrared range of spectra is more advanced than that of bulk crystalline Si.

Our finding can also shed light into the question as to why ion implanted, poly-, multi-crystalline and porous Si emits light better than bulk crystalline Si. According to traditional point of view the reason of more enhanced photoluminescence feature of the Si phases than unstrained bulk Si can been ascribed to dislocations.[8, 12, 13] If we suggest that voids can be formed upon ion implantation, or exist in poly-, multi-crystalline and porous Si then the regions with elongated Si-Si bonds could be formed around the voids. Those regions of Si can be direct band gap and radiative recombination of free carriers in these regions can be more enhanced than those in other unstrained ones.

The result as to well dispersive character of the bottommost CB at the Γ point and related small CB electron effective mass shows that the CB electron mobility can also be much larger than that at the *X* point of unstrained Si. This result can shed light into the recent finding as to the enhanced electrical conductivity through the channels formed by dislocations due to increase of carrier concentration and mobility.[38, 40]

It should be noted that the above mentioned applications of the features extracted from comparative analysis of band structure of strained Si can be important to extend device applications of Si also. For example, the feature of the strained Si to

posses CB minimum at the Γ point can be important for electric-field induced transfer of CB electrons from one valley into another. This has implications to use the strained Si as generator of ossillations similar to the well known GaAs one.[41]

Our finding that the origin of the PL is related to elongated Si-Si bond explains not only the reason of luminescence of porous, poly- and multi-crystalline, and dislocation engineered Si as well as a-Si:H, but also opens up another way of causing luminescent property of Si and enhancement of electrical conductivity by voids, since strains can be formed not only around dislocations, but also around multivacancies and voids. Then the distance between the Si atoms located in close vicinity of the multivacancy/void is expected to larger than that in the bulk. As it is well known multivacancies can be formed upon annealing of the Ar implanted Si.[42] This idea may have important technological consequences. If a nanowire is prepared from void and band gap of Si has been turned from indirect to direct, then electrical conductivity by CB electrons through such a wire is expected to be enhanced than that in bulk Si. This idea can present interest for photovoltaic solar cells. Luminescence properties of Si with nanodots from void or multivacancy complex then can be more superior than bulk Si. This point can be important for optoelectronic applications of Si. It has the implication that the Si with voids has the potential to be used as alternative to Er doped or dislocation engineered Si light-emitting diodes.

5. Conclusion

Thus we studied band structure of Si for different values of the lattice parameter, which corresponds to different strain values. It is found that in the strain range 0-20 GPa the topmost valence band remains at the Γ point. However, at strains from >12 GPa

bottommost conduction band is located at Γ point thus indicating that band structure of Si turns from indirect to direct. The bottommost conduction band at the Γ point of the strained Si is found to be much narrower than that at the X point of the bulk Si. Consequently, effective masses of the former are much smaller whereas electrical conductivity through it can be expected to be more superior than those of the latter. Barrier height needed to overcome for the electrons of the Γ point to be transferred into X/L points or from X/L to Γ point have been calculated. Since the regions in Si with strain and, consequently, elongated Si-Si bonds, can be formed in the close vicinity of the dislocation loops and voids, the origin of infrared luminescence of multi-, poly-, porous Si, a-Si:H as well as ion implanted Si are suggested to be related to modified band structure of Si from indirect to direct.

Acknowledgments

This work has received financial and supercomputing support from the Research Council of Norway through NANOMAT projects and from the Academy of Sciences of Uzbekistan.

References

[1] W. L. Ng, M. A. Lourenco, R. M. Gwilliam, S. Ledain, G. Shao, and K. P. Homewood, Nature **410**, 192 (2001).

[2] J. L. Corkill and M. L. Cohen, Phys. Rev. B **47**, 10304 (1993).

[3] E. A. Steinman, A. J. Kenyon, and A. N. Tereshchenko, Semicond. Sci. Technol. **23**, 025010 (2008).

[4] C. P. Ewels, S. Leoni, M. I. Heggie, P. Jemmer, E. Hernández, R. Jones, and P. R. Briddon, Phys. Rev. Lett. **84**, 690 (2000).

[5] M. I. Heggie, S. Jenkins, C. P. Ewels, P. Jemmer, R. Jones, and P. R. Briddon, J. Phys.:Condens. Matter **12**, 10263 (2000).

[6] O. V. Feklisova, E. B. Yakimov, N. A. Yarykin, and J. Weber, Mater. Sci. Eng. B **58**, 60 (1999).

[7] J. F. Justo, A. Antonelli, T. M. Schmidt, and A. Fazzio, Phys. B: Condens. Matter **273-274**, 473 (1999).

[8] A. G. Ulyashin, R. Job, W. R. Fahrner, A. V. Mudryi, A. I. Patuk, and I. A. Shakin, Mater. Sci. Semicond. Proc. **4**, 297 (2001).

[9] M. Kittler, X. Yu, T. McHedlidze, T. Arguirov, O. F. Vyvenko, W. Seifert, M. Reiche, T. Wilhelm, M. Seibt, O. Voss, A. Wolff, and W. Fritzsche, Small **3**, 964 (2007).

[10] N. A. Sobolev, B. Y. Ber, A. M. Emel'yanov, A. P. Kovarskii, and E. I. Shek, Semicond. **41**, 285 (2007).

[11] N. A. Sobolev, A. M. Emel'yanov, V. I. Sakharov, I. T. Serenkov, E. I. Shek, and D. I. Tetel'baum, Semicond. **41**, 537 (2007).

[12] A. V. Mudryi, A. I. Patuk, I. A. Shakin, A. G. Ulyashin, R. Job, W. R. Fahrner, A. Fedotov, A. Mazanik, and N. Drozdov, Sol. Energy Mater. Sol. Cells **72**, 503 (2002).

[13] A. V. Mudryi, F. P. Korshunov, A. I. Patuk, I. A. Shakin, T. P. Larionova, A. G. Ulyashin, R. Job, W. R. Fahrner, V. V. Emtsev, V. Y. Davydov, and G. Oganesyan, Physica B-Condens. Matter **308**, 181 (2001).

[14] R. A. Street, Adv. Phys. **30**, 593 (1981).

[15] T. Kruger, J. Appl. Phys. **99**, 063509 (2006).

[16] T. Kruger and A. F. Sax, Physica B-Condens. Matter **353**, 263 (2004).

[17] M. Ni, G. Luo, J. Lu, L. Lai, L. Wang, M. Jing, W. Song, Z. Gao, G. Li, W. N. Mei, and D. Yu, Nanotech. **18**, 505707 (2007).

[18] N.-M. Park, C.-J. Choi, T.-Y. Seong, and S.-J. Park, Phys. Rev. Lett. **86**, 1355 LP (2001).

[19] X. J. Zhu, S. Fahy, and S. G. Louie, Phys. Rev. B **39**, 7840 (1989).

[20] S. Fahy, K. J. Chang, S. G. Louie, and M. L. Cohen, Phys. Rev. B **35**, 5856 (1987).

[21] K. J. Chang, S. Froyen, and M. L. Cohen, Solid State Commun. **50**, 105 (1984).

[22] L. T. Canham, Appl. Phys. Lett. **57**, 1046 (1990).

[23] E. Ghahramani and J. E. Sipe, Phys. Rev. B **40**, 12516 (1989).

[24] P. S. Yadav, R. K. Yadav, S. Agrawal, and B. K. Agrawal, Prog. Cryst. Growth Charact. Mater. **52**, 10 (2006).

[25] G. Kresse and J. Hafner, Phys. Rev. B **47**, 558 (1993).

[26] G. Kresse and J. Furthmüller, Phys. Rev. B **54**, 11169 (1996).

[27] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. **77**, 3865 (1996).

[28] S. Z. Karazhanov, P. Ravindran, A. Kjekshus, H. Fjellvag, and B. G. Svensson, Phys. Rev. B **75**, 155104 (2007).

[29] J. E. Jaffe, M. Dupuis, and M. Gutowski, Phys. Rev. B (Condens. Matter Mater. Phys.) **69**, 205106 (2004).

[30] L. C. Lew Yan Voon, M. Willatzen, M. Cardona, and N. E. Christensen, Phys. Rev. B **53**, 10703 (1996).

[31] S. Karazhanov and L. Lew Yan Voon, Semicond. **39**, 161 (2005).

[32] in *Inorganic Crystal Structure Database* (Gmelin Institut, Karlsruhe, 2001).

[33] J. J. Hall, Physical Review **161**, 756 LP (1967).

[34] A. G. Beattie and J. E. Schirber, Phys. Rev. B **1**, 1548 LP (1970).

[35] Y. Ishibashi, T. Kobayashi, A. D. Prins, J. Nakahara, M. A. Lourenco, R. M. Gwilliam, and K. P. Homewood, Phys. Status Solidi B **244**, 402 (2007).

[36] B. Welber, C. K. Kim, M. Cardona, and S. Rodriguez, Sol. State Commun. **17**, 1021 (1975).

[37] B. Freytag, Semiconductor Science and Technology **10**, 270 (1995).

[38] M. Kittler, M. Reiche, T. Arguirov, T. Mchedlidze, W. Seifert, O. F. Vyvenko, T. Wilhelm, and X. Yu, Sol. State Phenom. **131-133**, 289 (2008).

[39] T. Mchedlidze, T. Arguirov, M. Kittler, T. Hoang, J. Holleman, P. LeMinh, and J. Schmitz, Sol. State Phenom. **131-133**, 303 (2008).

[40] T. Mchedlidze, T. Wilhelm, T. Arguirov, G. Jia, M. Reiche, and M. Kittler, Solid State Phenomena **131-133**, 503 (2008).

[41] P. Yu and M. Cardona, *Fundamentals of Semiconductors: Physics and Materials Properties* (Springer-Verlag, Berlin And Heidelberg Gmbh & Co. Kg, 2005).

[42] A. G. Ulyashin, R. Job, W. R. Fahrner, A. V. Mudryi, A. I. Patuk, and I. A. Shakin, in *High purity Silicon VI*, edited by C. L. Claes, P. Rai-Choudhary, M. Watanabe, P. Stallhofer and H. J. Dawson (SPIE - The International Society for optical engineering, 2000), Vol. 2000-17, p. 66.

[43] A. K. Walton and P. L. Reimann, J. Phys. C: Solid State Phys. **3**, 1410 (1970).

[44] J. C. Hensel and G. Feher, Phys. Rev. **129**, 1041 (1963).

[45] P. Lawaetz, Phys. Rev. B **4**, 3460 (1971).

Table I. Calculated by DFT and determined experimentally electron (m_c) and hole (m_h) effective masses (in units of the free electron mass m_0) for bulk and strained Si.

Compound	P	m_c	m_h
Si, Theory	0	1.09 (X)	0.27 (Γ→X), 0.79 (Γ→L)
Si, Exp	0	1.08[a](X)	0.217[b] (Γ→X) 0.541[c] (Γ→L)
Si	12.65	0.05 (Γ)	0.27 (Γ→X) 0.77 (Γ→L)

[a]) Experiment.[43]

[b]) Experiment. [44]

[c]) k.p theory, semiempirical results.[45]

Figure captions

Fig. 1. Band structure for Si strained with P=0.0 and 11.9 GPa. Fermi level is set at zero energy.

Fig. 2. Indirect band gap related to *L* and *X* points as well as direct band gap for Si as a function of straining pressure calculated from DFT.

Fig. 3. Fundamental band gap of Si as a function of straining pressure. The results have been compared to the experimentally measured pressure dependence of the optical absorption edge[36] and photoluminescence peak energy.[35]

Fig. 4. Barrier height to transfer of an electron from the extremum at *L*,*X* points to Γ and from the extremum at the Γ to *L*,*X* points.

Fig. 5. Valence band offset between strained parts of Si. Topmost VB of unstrained Si is set to zero. CB offset has been estimated using the band gap values of strained Si calculated[24] by GW approximation.

Fig. 6. Si-Si bond length and primitive unit cell volume of Si as a function of the strain. Theoretical results have been presented by symbols and continuous lines correspond to fitting by 6^{th} order polynom for Si-Si bond length and 3^{rd} order polynom for volume of the primitive unit cell.

Fig. 7. Schematic presentation of a quantum (a) dot and (b) wire in Si consisting of a void.

Fig. 8. Number of Si-Si bonds as a function of the Si-Si bond length for (a) primitive unit cell of Si with relaxed (open bars) and unrelaxed lattice (solid bars) as well as for Si supercell with a void in the form of a (b) dot and (c) wire.

Fig. 9. Band structure for Si with a quantum (i) dot and (b) wire consisting of a void. Fermi level is set at zero energy.